Supervised Learning

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Overview

- What is supervised learning?
- Cross-validation
- k-nearest neighbour (kNN)
- Decision trees
- Random forests
- Support vector machines

What's the problem?

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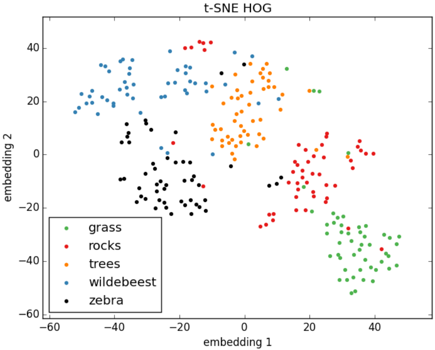
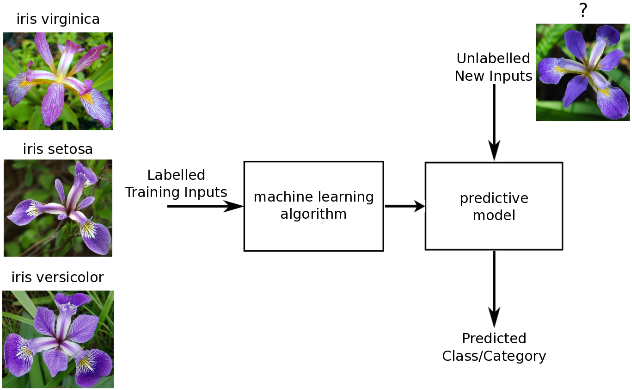
https://www.livescience.com/23310-serengeti.html

Counting wildebeest



What is supervised learning?

Supervised learning methods determine the mapping (**predictive model**) between a set of features and a continuous outcome (**regression**), or a categorical variable (**classification**)



Bias-variance tradeoff

- Machine learning algorithms are very flexible in order to deal with complex data
- So how *well* should we fit to the training data to get good generalisation?
- Driving the training error to zero is *not* a good idea

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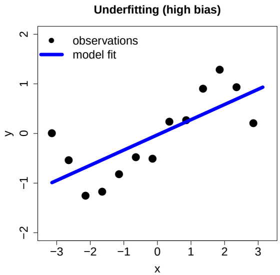

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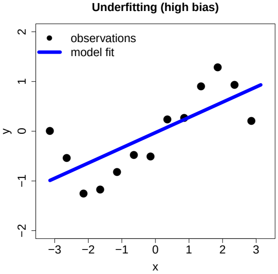

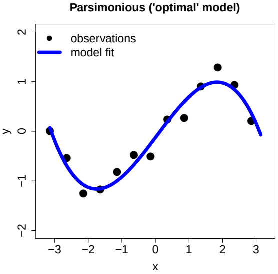

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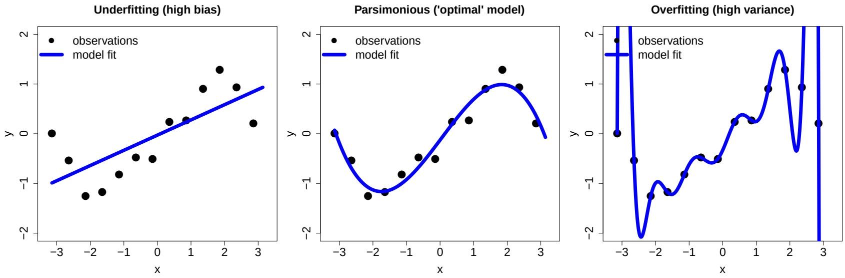

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- The flexibility of ML models is constrained by **tuning** their **hyperparameters**
- k-**fold cross-validation** allow us to find optimal hyperparameters

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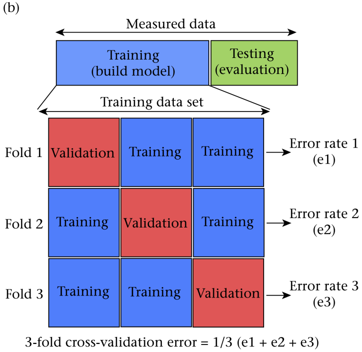
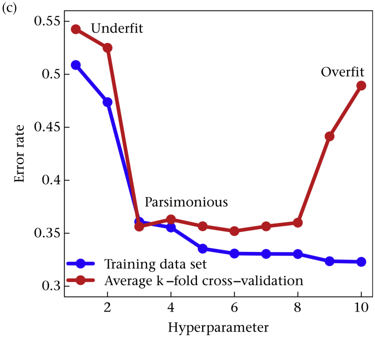
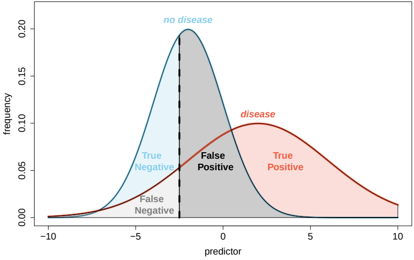
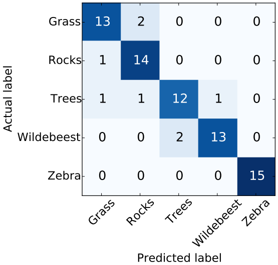




Predictive performance measures

- To compare models during cross-validation **predictive performance measures** are computed
- Several metrics exist, some of the more popular ones are:
  - **Regression**: root mean squared error (RMSE), R-squared
  - **Classification**: area uder the ROC curve, confusion matrix





k-nearest neighbour (kNN)

1. Calculate distance between test point and every training data point
2. Find the k training points closest to test point
3. Assign test point the majority vote of their class label

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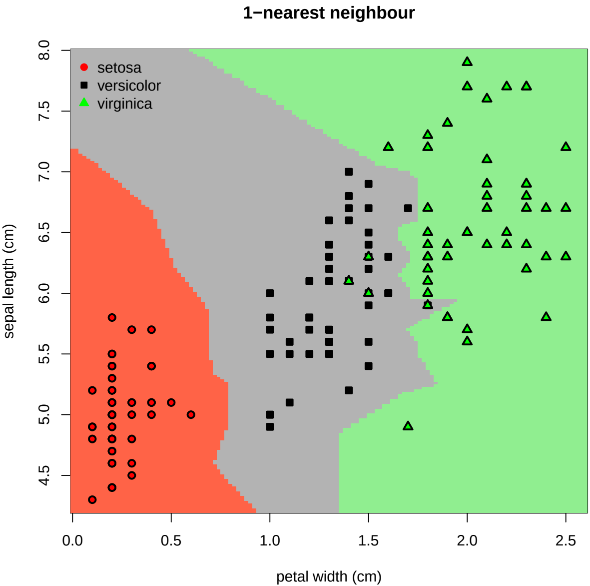

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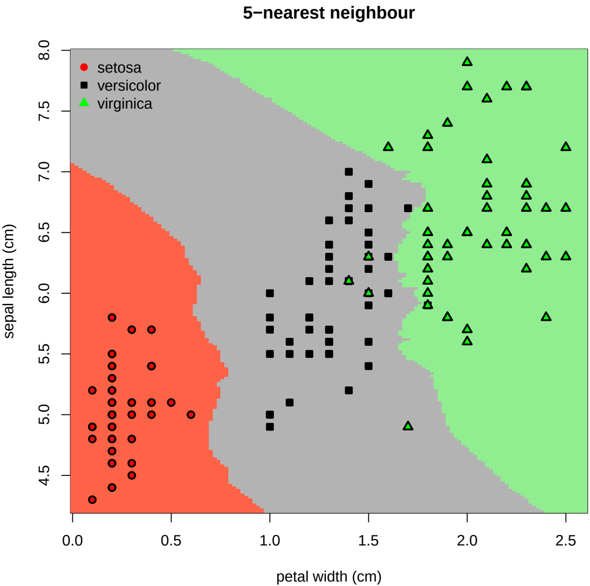

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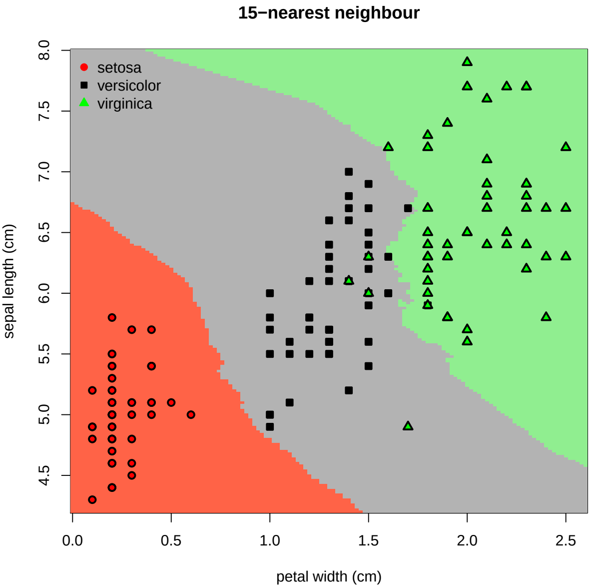

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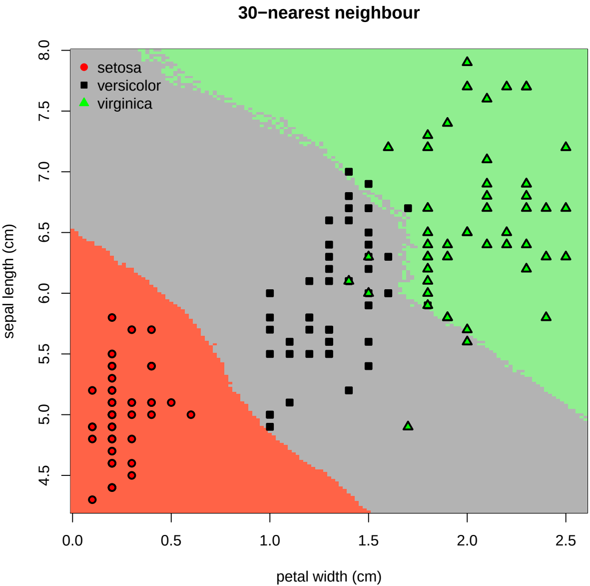

k-nearest neighbour

Pros

- Simple and intuitive
- Works for multi-class problems
- Non-linear decision boundaries
- k easily tuned by cross-validation

Cons

- Can be computationally expensive, as for every test point, distance to *every* training data point needs to be computed
- Takes up a lot of storage as *all* training points need to be retained

Decision trees

1. Find the yes/no rule that best splits the data with respect to *one* of the features

2. The best split is the one that produces the most homogeneous groups; found by maximising information gain/lowering entropy.

3. Repeat steps 1 to 2 until all data are correctly classified or some stopping rule reached.

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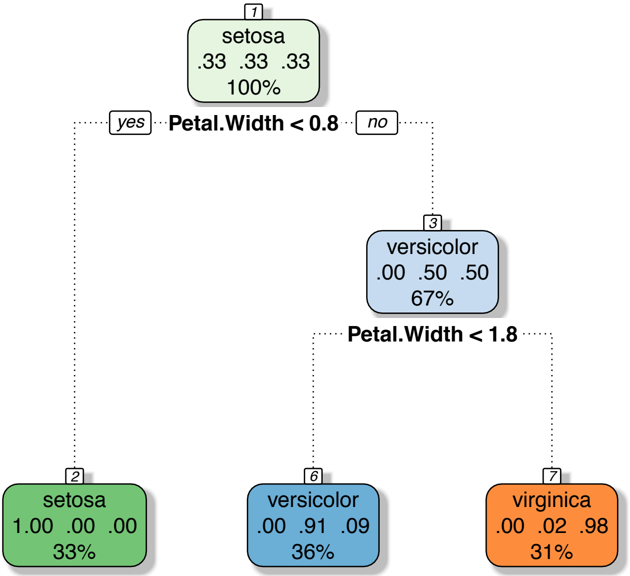
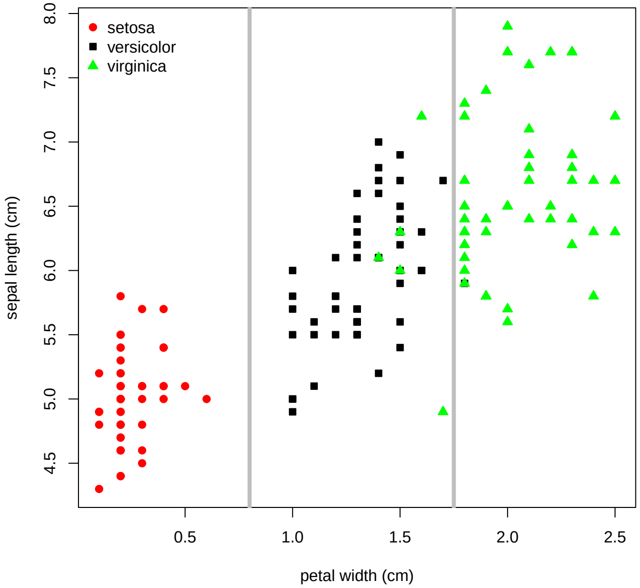


Decision boundaries



Decision trees

Pros

- Model is very easy to explain to non-experts and can be directly used to generate rules
- Computationaly inexpensive to train, evaluate and store
- Handle both categorical and continuous data
- Robust to outliers

Cons

- Can easily overfit the data
- Predictive accuracy can be poor
- Linear decision boundaries
- Small changes to training data may lead to a completely different tree

Random forests

- Decision trees are intuitive but suffer from overfitting which significantly affect their predictive accuracy
- **Pruning**, to "trim" the tree back, help reduce this overfit
- **Ensemble** methods such as Random Forests are a better alternative
- **Rationale**: Instead of one tree, grow a *forest*, where every bushy tree (no pruning) is a bit different, then average predictions over all trees

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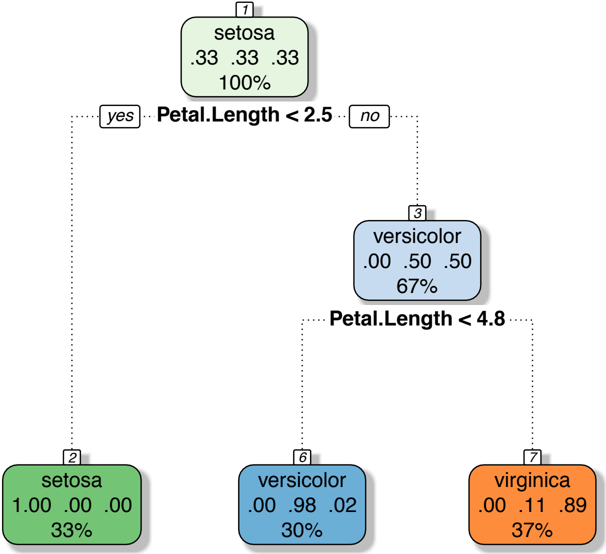

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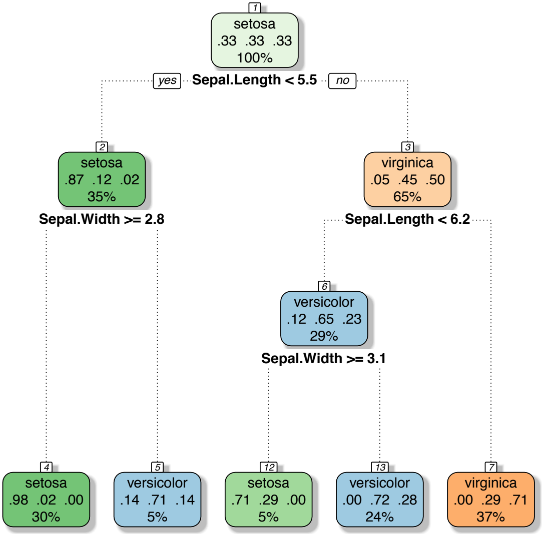
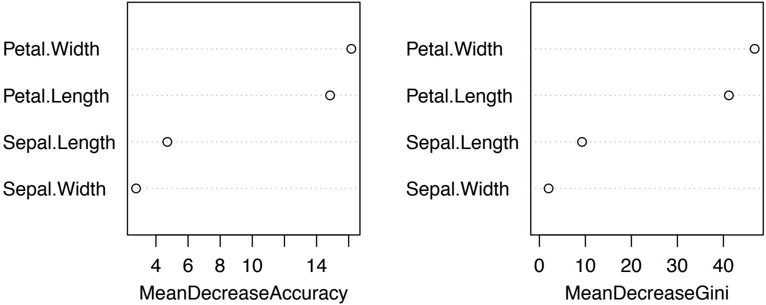


Variable importance

- Cannot visualise decision boundaries (loss of interpretability)

- However, variable importance helps us perform feature selection



Random forests

Pros

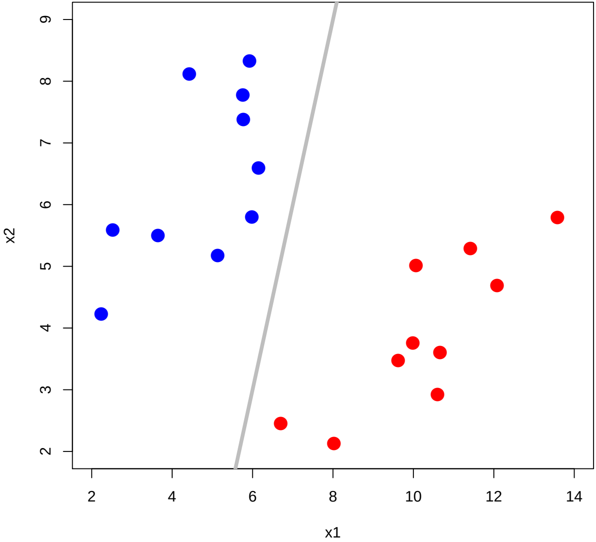
- State-of-the-art predictive accuracy
- Can handle thousands of both categorical and continuous predictors without variable deletion
- Robust to outliers
- Estimates the importance of every predictor
- Out-of-bag error (unbiased estimate of test error for every tree built)
- Can cope with unbalanced datasets by setting class weights
- Trivially parallelisable

Cons

- Harder to interpret then plain decision trees

Support vector machines (SVMs)

Which is the best separating line?



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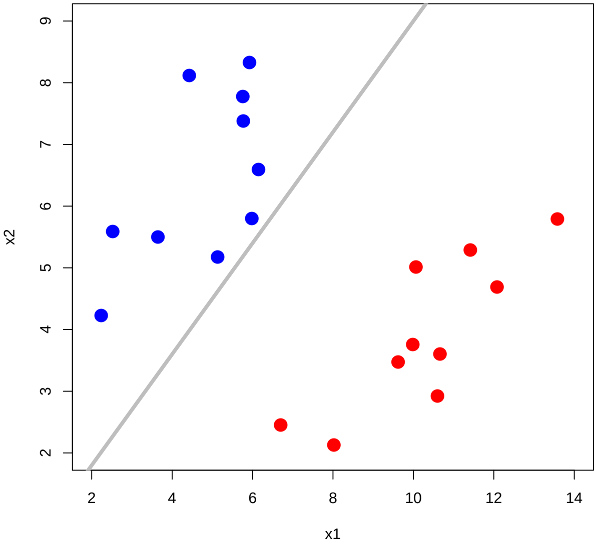

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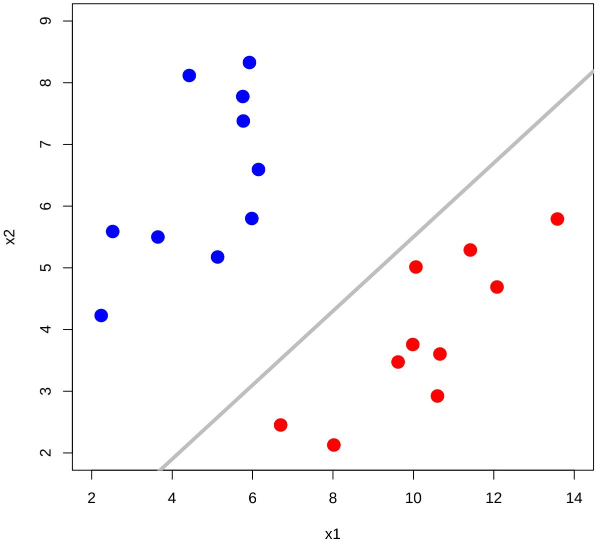

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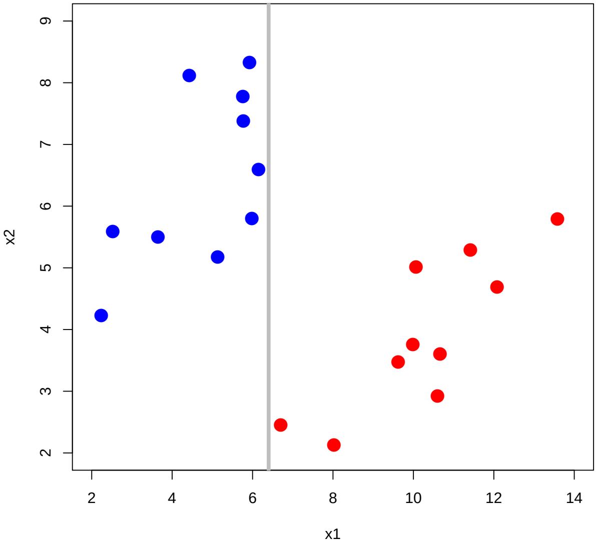
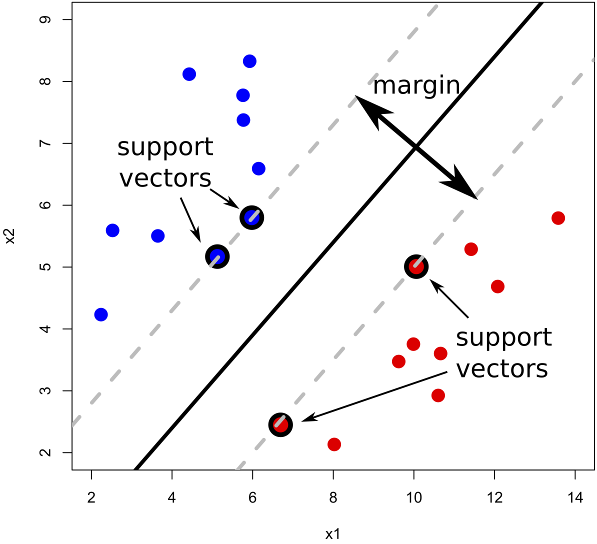
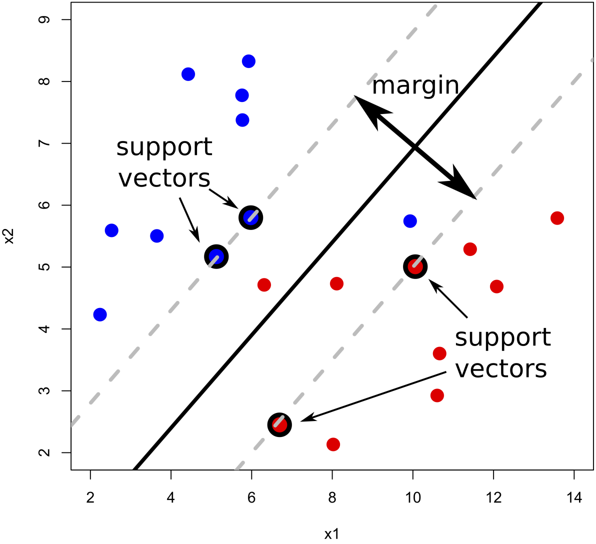


Maximal margin classifier

Rationale: Maximise the *margin*

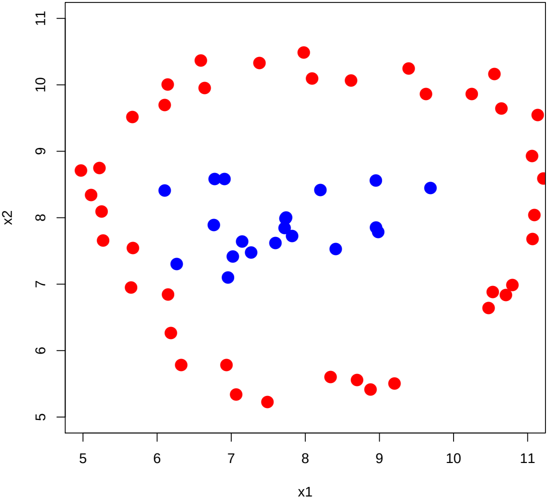


Rationale: Use a *soft* margin



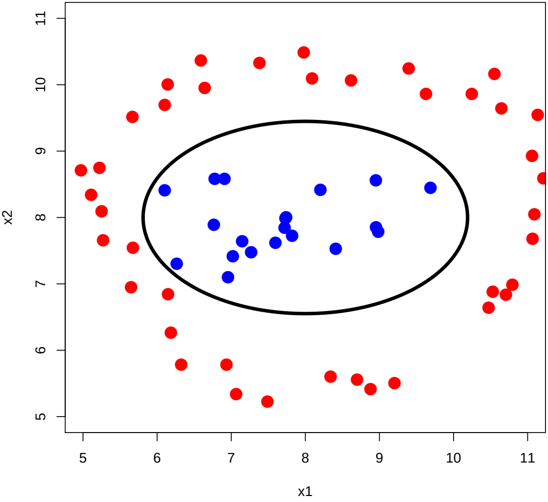
Support vector machines

Real-life data is complex and often we cannot find a separating hyperplane

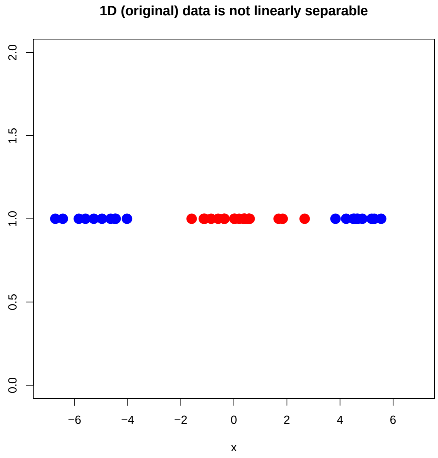


Support vector machines

Rationale: Map data to a higher dimensional space where classes are linearly separable



Support vector machines: 1D to 2D



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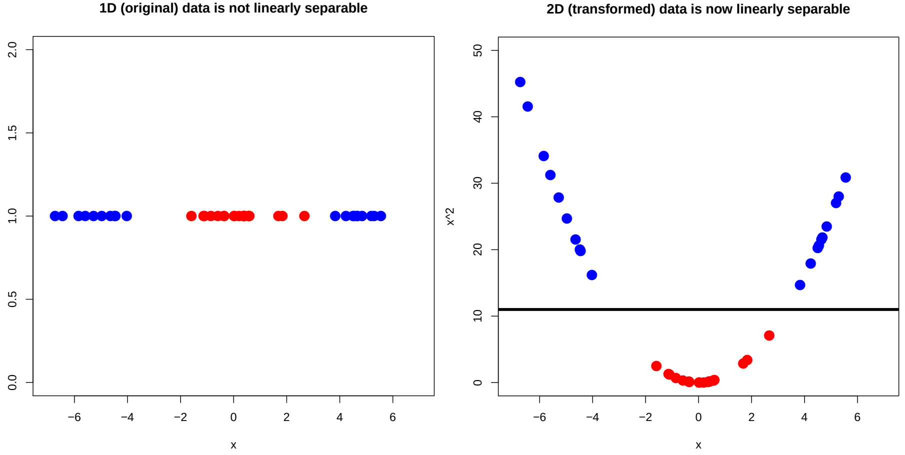

Support vector machines - the kernel trick

- So our solution is to blow up the dimensions?
- But what about the “curse of dimensionality”?
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- Very computationally expensive to work in high dimensions

- **Kernel trick** to the rescue!
- Work in an *implict* feature space
- Data is never explicitly computed in higher dimensions
- Think about kernels as generalised distance measures

p.s Kernel methods are mathematically intricate and beyond the scope of this introductory workshop

Support vector machines

1. Choose a kernel

2. Run optimiser to find the maximum margin separating hyperplane

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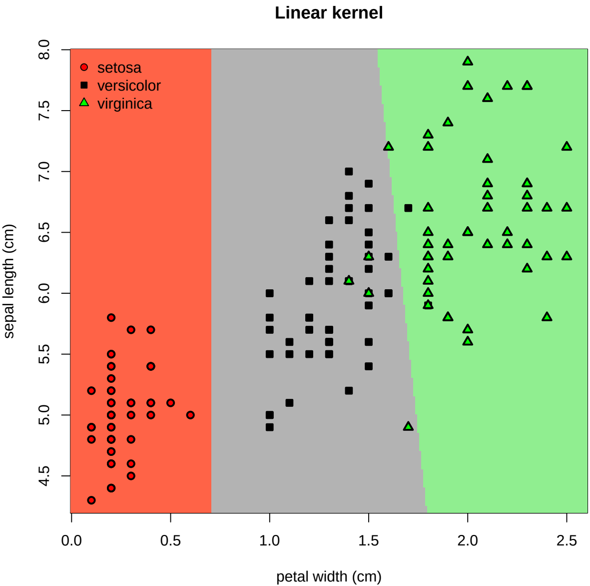
SVMs are inherently binary classifiers. The most common ways to deal with multi-class problems is by building several **one-versus-all** *or* **one-versus-one** classifiers.

Support vector machines



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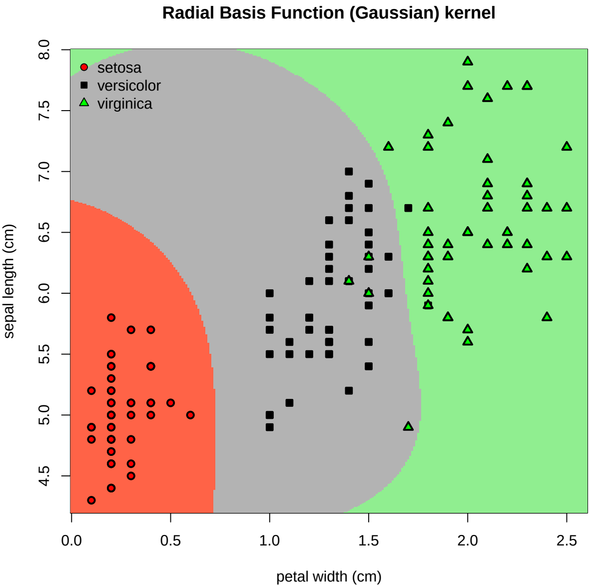

Support vector machines

Pros

- State-of-the-art predictive accuracy
- Low storage requirements (only support vectors to store)
- A vast array of kernels are available that are flexible enough to cater for any type of data
- Global optimum guaranteed

Cons

- Model is hard to interpret
- Feature space cannot be visualised